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United States Environmental Protection Agency
Washington, DC 20460

E. White

ORIGINAL

Document Description

SAT L-07-293

Date

7/20/07

STRUCTURE ACTIVITY TEAM REPORT

ver. 04/98

Case #: L-07-0293

DCN:

SAT Date: 6/29/2007

SAT Chair:

V. Nabholz

Submitter: Tracerco

Chemical Name:

Benzoic acid, 2,5-difluoro-, sodium salt (1:1)

CAS RN:

522651-42-9

Trade Name:

Tracerco 158I

Structure



6 0 0 7 0 0 0 2 1 6 5

Molecular Formula:

 $\text{C}_7\text{H}_3\text{F}_2\text{NaO}_2$

Molecular Wt. 180

WT%<500:

WT%<1000:

MP:

BP:

>500

Eq. Wt:

H₂O Sol (g/L):

>200

V.P.

<0.000001

Max. Prod. Volume (kg/yr):

500

Physical State:

Solid

USE:

Tracer chemical to measure flow in deep oil-bearing strata. Concurrently submitted similar cases L-07-290 and L-07-292 to L-07-295. Analog L-07-271 has this same use. There is one reference in file CA on STN, a toxicity study.

P2REC: CRSS: forward. P2 Claim: The LVE substance is a substitute for radionuclide tracers to measure the flow rate in oil-bearing strata. The LVE substance has been awarded Offshore Chemical Notification System Gold Band Status by European regulatory authorities.

Related Case Numbers	Case Role	Related Case Numbers	Case Role

Focus Date: JUL 9 2007

Results:

Conditional Grant

P2REC →

STRUCTURE ACTIVITY TEAM REPORT 29 June 2007

CASE NUMBERS: L07-0290 to L07-~~0330~~³⁰⁰

L07-0290 (F2)
L07-0291 (F)
L07-0292 (F2)
L07-0293 (F2)
L07-0294 (F2)
L07-0295 (F2)
L07-0296 (F4)
L07-0297 (F3)
L07-0298 (CF3)
L07-0299 (CF3)
L07-0300 (CF3)

P2REC: substitute for radionuclide tracers

RELATED CASES:

L07-0271 (F)



CONCLUSIONS/DISCUSSIONS

TYPE OF CONCERN: HEALTH ECOTOX

LEVEL: 1-2 1

KEYWORDS: DEVEL, LIVER, KIDNEY, SENS-ASTHMA, MUTA

SUMMARY OF ASSESSMENT:

FATE: MW162 to 216
solids with mp for L070271 (F) = 126 °C (M)
log Kow for the free acid = 1.8 to 2.9 (ClogP), 1.2 to 2.8 (EPI),
1.59 to 3.10 (M)
log Kow for L070271 = -5.87 with pH? (HPLC)
log Kow for L070296 = -2.11 with pH? (HPLC)
log Kow for L070297 = -3.62 with pH? (HPLC)
log Kow for L070298 = -1.64 with pH? (HPLC)
S > 200 mg/L to > 10 g/L at 20 °C (P)
vp < 1.0E-6 mm Hg or torr at 25 °C (P)
bp = 460 °C (P)
H for the covalent ion pair = 1.2E-7 to 9.5E-7 (P)
log Koc for the covalent ion pair = 1.4 to 2.0 (P)
log fish BCF = 0.50 (P)
sorption to sludge = low (P)

test data for L070271 for aerobic biodegradation in seawater at 20 C, via closed bottle (OECD306) were:

time	biodegradation
(d)	(percent)
5	0
14	2
28	63

test data for aerobic biodegradation for the [REDACTED] of L070299 from [REDACTED] were:

15% biodegradation in 28 d, thus, not readily biodegradable via CO₂ evolution in modified Sturm test (OECD301B); if test result is due solely to ester hydrolysis and degradation of the [REDACTED] moiety, then removal via POTW of the parent would be >= 90% but notifier did not measured degradation products;

POTW removal = 0% to 90 via sorption and possible biodegradation time for complete ultimate aerobic biodegradation = weeks to => months

sorption to soils and sediments = low (P)

PBT Potential: P2B1T2 to P3B1T2

*CEB FATE: migration to ground water = rapid

HEALTH: Absorption nil thru skin based on physical/chemical properties; good thru lungs based on analogs; and good thru the GI tract based on analogs;

test data for the [REDACTED] of L070299, [REDACTED], were:

rat acute oral LD₅₀ = 800 mg/kg with toxic signs; LD₁₀₀ = 2 g/kg, LD₀ = 300 mg/kg;

rat acute dermal LD₀ = 2.0 g/kg with no toxic signs; slight and transient (2 d) skin irritation in rabbits; slight and transient (1 d) eye irritation in rabbits; Ames test was negative;

E. coli test was negative;

chromosome aberration test with V79 cells was positive with activation, but negative without activation; no skin sensitization in guinea pigs (M&K);

rat 28-d subchronic oral-gavage with doses = 1000, 300, and 100 mg/kg/d with NOAEL = 100 mg/kg/d and LOEL = 300 mg/kg/d based on salivation and increased water consumption; effects at 1000 mg/kg/d were slight to severe salivation, unsteady gait, motor activity significantly decreased and effects to the liver and kidneys;

concern for asthma and developmental toxicity based on data for benzoic acid, note: the mechanism for the asthma is unknown;

concern for possible mutagenicity, liver toxicity, and kidney toxicity based on data for [REDACTED] which was the [REDACTED] of L070299, however, the [REDACTED] will have some acylating activity

which is absent in the acid, thus, the acid will be less toxic than the [REDACTED];

low to moderate concern for toxicity

*CEB HEALTH: Exposures to humans: inhalation, ingestion, and drinking water;

ECOTOX: Predicted (P) and measured (M) toxicity values in mg/L (ppm) are:

fish 96-h LC50	>	100.0	P
SW fish 96-h LC50	=	440.0	M S,N L070271
SW fish 96-h LC50	>	320.0	M S,N L070290
SW fish 96-h LC50	>	320.0	M S,N L070291
daphnid 48-h LC50	>	100.0	P
SW invert Ac ton 48-h LC50	=	2830.0	M S,N L070271
SW invert Ac ton 48-h LC50	=	1500.0	M S,N L070290
SW invert Ac ton 48-h LC50	=	430.0	M S,N L070291
SW invert Ac ton 48-h LC50	=	480.0	M S,N L070292
SW invert Ac ton 48-h LC50	=	270.0	M S,N L070293
SW invert Ac ton 48-h LC50	=	250.0	M S,N L070294
SW invert Ac ton 48-h LC50	=	250.0	M S,N L070295
SW invert Ac ton 48-h LC50	=	300.0	M S,N L070296
SW invert Ac ton 48-h LC50	=	430.0	M S,N L070297
SW invert Ac ton 48-h LC50	=	440.0	M S,N L070298
SW invert Ac ton 48-h LC50	=	170.0	M S,N L070299
SW invert Ac ton 48-h LC50	=	130.0	M S,N L070300
green algal 96-h EC50	>	100.0	P
SW algae Sk cost 72-h EC50 c	=	250.0	M S,N L070271
SW algae Sk cost 72-h EC50 r	>	10000.0	M S,N L070290
SW algae Sk cost 72-h EC50 r	=	430.0	M S,N L070291
SW algae Sk cost 72-h EC50 r	=	660.0	M S,N L070292
SW algae Sk cost 72-h EC50 r	=	2100.0	M S,N L070296
SW algae Sk cost 72-h EC50 r	=	1500.0	M S,N L070297
SW algae Sk cost 72-h EC50 r	=	700.0	M S,N L070300
fish chronic value	>	10.0	P
daphnid ChV	>	10.0	P
algal ChV	>	10.0	P
SW algae Sk cost ChV c	=	100.0	M S,N L070271
SW algae Sk cost ChV r	=	5600.0	M S,N L070290
SW algae Sk cost ChV r	<	100.0	M S,N L070291
SW algae Sk cost ChV r	=	320.0	M S,N L070292
SW algae Sk cost ChV r	=	1000.0	M S,N L070296
SW algae Sk cost ChV r	=	320.0	M S,N L070297
SW algae Sk cost ChV r	=	320.0	M S,N L070300
benthic			
SW invert Coror vol 10-d LC50	=	6558.0	mg/kg DWT M S,N L070271
SW invert Coror vol 10-d NOEC	=	470.0	mg/kg DWT M S,N L070271
SW invert Coror vol 10-d LC50	=	7300.0	mg/kg DWT M S,N L070290
SW invert Coror vol 10-d NOEC	=	1400.0	mg/kg DWT M S,N L070290
SW invert Coror vol 10-d LC50	=	3800.0	mg/kg DWT M S,N L070291
SW invert Coror vol 10-d NOEC	=	150.0	mg/kg DWT M S,N L070291

SW invert Coror vol 10-d LC50	=	6700.0	mg/kg DWT M S,N L070292
SW invert Coror vol 10-d NOEC	=	1400.0	mg/kg DWT M S,N L070292
SW invert Coror vol 10-d LC50	=	410.0	mg/kg DWT M S,N L070296
SW invert Coror vol 10-d NOEC	=	130.0	mg/kg DWT M S,N L070296
SW invert Coror vol 10-d LC50	=	330.0	mg/kg DWT M S,N L070297
SW invert Coror vol 10-d NOEC	=	160.0	mg/kg DWT M S,N L070297
SW invert Coror vol 10-d LC50	=	280.0	mg/kg DWT M S,N L070300
SW invert Coror vol 10-d NOEC	=	16.0	mg/kg DWT M S,N L070300

Predictions are based on SARs for neutral organic chemicals with 10X less toxicity due to the substitution of the acid, or SARs for anionic surfactants-carboxylic acid-C4.Na; SAR chemical class = surfactant-anionic-F1 to F4 and CF3 benzene-COO.Na; MW162 to 216; solids with mp for L070271 (F) = 126 °C (M); log Kow for the free acid = 1.8 to 2.9 (ClogP), 1.2 to 2.8 (EPI), 1.59 to 3.10 (M); log Kow for L070271 = -5.87 with pH? (HPLC); S > 200 mg/L at 20 °C (P); pH7; effective concentrations based on 100% active ingredients and mean measured concentrations; hardness <150.0 mg/L as CaCO₃; and TOC <2.0 mg/L; low concern for toxicity

assessment factor = 10.0

concern concentration = 1.0 mg/L (ppm)

*CEB ECOTOX: No releases to water;

P2REC: forward to FOCUS with support.

SAT Co-chair: Vince Nabholz, 564.8909

GTOX Report

PMN No. L-07-0293 CAS No. 522651-42-9 Rcvd: 06/18/07 OECD Incomplet ID: Rec# 4 : 857
S/A Name of Analog S [Redacted] Reviewer ked

	with activation	without activation	Positive Strains
Salmonella Assay:	<input type="checkbox"/>	<input type="checkbox"/>	[Redacted]
Chromosomal Aberration	CHO: <input type="checkbox"/>	<input type="checkbox"/>	
	CHL: <input type="checkbox"/>	<input type="checkbox"/>	
	V79: <input type="checkbox"/>	<input type="checkbox"/>	
E. coli Reverse Mutation:	<input type="checkbox"/>	<input type="checkbox"/>	
Mouse Micronucleus Assay:	Route: [Redacted]	<input type="checkbox"/>	
Rat Hepatocytes Unscheduled DNA Synthesis:		<input type="checkbox"/>	

Other GTOX Results

[Large empty box for Other GTOX Results]

Comments

[Large empty box for Comments]

ECOTOX:**Fate:**

[Large empty box for Fate]

WS/Log P:

[Large empty box for WS/Log P]

NCSAB SAT REPORT

C [REDACTED] N

PMN: L-07-0293

CAS RN:

522651-42-

Chemical Name:

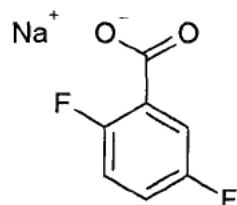
Benzoic acid, 2,5-difluoro-, sodium salt (1:1)

Analogs:

Production Volume:

500.0

Structure:

User chemical to measure flow in deep oil-bearing strata.

Concurrently submitted similar cases L-07-290 and L-07-292 to L-07-295.

Analog L-07-271 has this same use. There is one reference in file CA on STN, a toxicity study.

P2REC: CRSS: forward. P2 Claim: The LVE substance is a substitute for radionuclide tracers to measure the flow rate in oil-bearing strata. The LVE substance has been awarded Offshore Chemical Notification System Gold

Formula:	C ₇ H ₃ F ₂ NaO ₂	Eq Wt:
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Mol Weight:	180.09	Wt%<500:	Wt%<1000
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MP:		BP:	>500	VP:	<0.000001
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H ₂ O Sol (g/L):	>200	Physical State:	Solid	Log P:
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Endpoint (mg/L)	Est. Value	Meas. Value	Comments
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Fish 96-h			
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Daphnid 48-h			
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Algal 96-h			
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Fish ChV			
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Daphnid ChV			
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Algal ChV			
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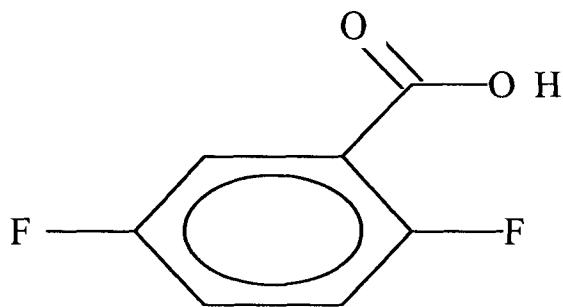
BCF			
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CHEMICAL CLASS:	SAR:		
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ECOTOX CONCERN	H	M	L	CONCERN CONCENTRATION
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DATE	ASSESSOR:		
------	-----------	--	--

L-07-293



SMILES : Fc1ccc(F)cc1C(=O)(O)
 CHEM :
 CAS Num:
 ChemID1:
 ChemID2:
 ChemID3:
 MOL FOR: C7 H4 F2 O2
 MOL WT : 158.11
 Log Kow: 2.04 (User entered)
 Melt Pt: 134.00 deg C
 Wat Sol: 210 mg/L (calculated)

ECOSAR v0.99h Class(es) Found

 Neutral Organics-acid

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	: Fish	14-day	LC50	195.932

--> Acid moiety found: Predicted values multiplied by 10

Neutral Organics-acid	: Fish	96-hr	LC50	1074.847 *
Neutral Organics-acid	: Fish	14-day	LC50	1959.325 *
Neutral Organics-acid	: Daphnid	48-hr	LC50	1154.906 *
Neutral Organics-acid	: Green Algae	96-hr	EC50	723.680 *
Neutral Organics-acid	: Fish	30-day	ChV	139.363
Neutral Organics-acid	: Daphnid	16-day	EC50	60.276
Neutral Organics-acid	: Green Algae	96-hr	ChV	74.060
Neutral Organics-acid	: Fish (SW)	96-hr	LC50	251.042 *
Neutral Organics-acid	: Mysid Shrimp	96-hr	LC50	301.263 *

Neutral Organics-acid	: Earthworm	14-day	LC50	mg/kg (ppm) dry wt soil
				=====
				9454.235 *

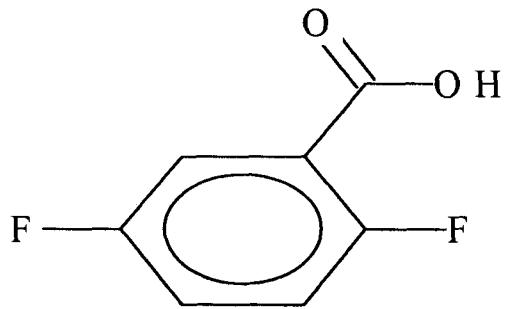
Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect.

Fish and daphnid acute toxicity log Kow cutoff: 5.0

Green algal EC50 toxicity log Kow cutoff: 6.4

Chronic toxicity log Kow cutoff: 8.0

MW cutoff: 1000



SMILES : Fc1ccc(F)cc1C(=O) (O)

CHEM :

MOL FOR: C7 H4 F2 O2

MOL WT : 158.11

----- EPI SUMMARY (v3.12) -----

Physical Property Inputs:

Water Solubility (mg/L) :	-----	Log Kow (oct-water):	2.04
Vapor Pressure (mm Hg) :	-----	Boiling Pt (deg C):	-----
Henry LC (atm-m3/mole) :	-----	Melting Pt (deg C):	134.00

Log Kow (KOWWIN v1.67 estimate) = 1.93

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1.41):

Boiling Pt (deg C):	241.34
Melting Pt (deg C):	47.62
VP(mm Hg, 25 deg C):	0.00333

Water Solubility estimate (WSKOW v1.41): 2149 mg/L

Water Solubility estimate (fragments): 6599.1 mg/L

Henry's Law Constant (atm-m3/mole) [HENRYWIN v3.10]:

Bond Method:	1.48E-007	Group Method:	3.62E-007
Henry's LC [VP/WSol estimate using EPI values]: 3.224E-007 atm-m3/mole			

Biodegradation Estimates (BIOWIN v4.02):

Atmospheric Oxidation (25 deg C) [AopWin v1.91]:

OH Half-Life =	12.961 Days (12-hr day; 1.5E6 OH/cm3)
No Ozone Reaction Estimation	

Soil Adsorption (PCKOCWIN v1.66): Koc = 38.81 Log Koc = 1.589

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1.67]:

Rate constants can NOT be estimated for this structure!

BCF estimate (BCFWIN v2.15): Log BCF = 0.500 (BCF = 3.162)

Volatilization from Water: (Henry LC = 3.62e-007 atm-m3/mole)
Half-Lives: Model River = 2035 hr, Model Lake = 2.231e+004 hr

Removal In Wastewater Treatment (percents, 99% recommended maximum):
TOTAL: 2.30, Biodeg: 0.10, Sludge: 2.19, Air: 0.02

Level III Fugacity Model (conc %, half-life hr):

Air(1.33%,311), Water(26.1%,1.44e+003), Soil(72.4%,2.88e+003), Sediment(0.108%,1.3e+004)
Persistence Time: 1.38e+003 hr

CHEMICAL: Unknown
MOL WT : 158.11
MOL FOR: C7H4F2O2
SMILES : Fc1ccc(F)cc1C(=O)=O
ISOC-ID: -a-aaa---aa---
FRAG-ID: 1_____2_____3_3_3
H-COUNT: _____11____1____1

10:19:01 06/27/:7

Class	Type	Contribution Description	Comment	value
FRAGMENT	# 1	Fluoride	MEASURED	0.370
FRAGMENT	# 2	Fluoride	MEASURED	0.370
FRAGMENT	# 3	Carboxy (ZW-)	MEASURED	-0.030
ISOLATING	CARBON	6 Aromatic isolating carbon(s)		0.780
EXFRAGMENT	HYDROG	3 Hydrogen(s) on isolating carbons		0.681
ELECTRONIC	SIGRHO	2 Potential interactions; 1.50 used	withinRing	0.147
ORTHO	RING 1	1 Normal ortho interaction(s)		-0.280
RESULT	v3.3	All fragments measured	ESTIMATE	2.038

ATTENDEES

SIGNATURE

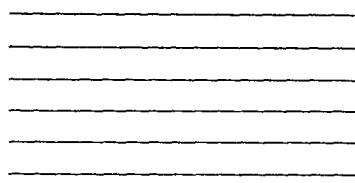
CHEMISTRY

- Paul Bickart
 Diana Darling
 Rich Engler
 Greg Fritz
 Daniel Lin
 Kathy Schechter



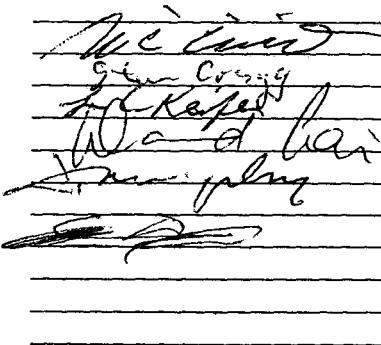
ENVIRONMENTAL FATE

- Bob Boethling
 Wen-Hsiung Lee
 Laurence Libelo
 David Lynch
 Andy Mamantov



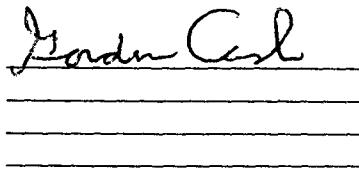
HEALTH

- Katherine Anitole
 Michael Cimino
 Steve Cragg
 Leonard Keifer
 David Lai
 Jim Murphy
 Deborah Norris
 Ronald Ward
 Yin Tak Woo



ENVIRONMENTAL EFFECTS

- Gordon Cash
 Vince Nabholz
 Maggie Wilson



SAT CHAIR/OTHER

- Rebecca Jones
 Leonard Keifer
 Vince Nabholz
 Jim Kwiat

